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This project has covered a number of areas related to theoretically modelling FEL laser interactions with materials. In particular we have been interested in developing models for incorporation or the essential aspects of the laser interactions into a molecular dynamics (MD) model as the MD approach provides a microscopic picture of atomic motions.

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This project has covered a number of areas related to theoretically modeling FEL laser interactions with materials. In particular we have been interested in developing models for incorporation or the essential aspects of the laser interaction into a molecular dynamics (MD) model as the MD approach provides a microscopic picture of atomic motions. Since this project has spanned seven years, we will concentrate on the most recent work in this report.

The highlight of our accomplishments is the recent development of a breathing sphere model for laser ablation of solids. The essence of this model is to treat each molecule (rather than an atom) as the particle of interest in the simulation. In addition to the traditional translational degrees of freedom, though, the molecules can breathe or change size. This allows us to incorporate realistic rates of energy transfer from individual molecules to the surrounding material. Specific properties of the laser such as pulse width, wavelength, fluence can be incorporated. In addition, heterogeneous samples can be modeled. The highlights to date are given below.

- The microscopic mechanisms of laser ablation are delineated. The laser induced pressure buildup and the phase explosion due to overheating of the irradiated material are identified as the key processes that determine the dynamics of laser ablation.

- The fluence threshold behavior in laser ablation is predicted. The physics of the material removal below and above threshold is analyzed.

- An expression for the analytical description of the velocity distribution in laser ablation is proposed based on the simulation results.

- Conditions for desorption of large analyte molecules in matrix assisted laser desorption (MALDI) are studied. The existence of the fluence threshold for the ejection of analytes, high kinetic energies and weak mass dependence of the ejection velocities on the molecular mass as well as the conditions that provide survivability of large fragile biomolecules in MALDI are addressed.

- Photomechanical the thermal damage mechanisms within adsorbing granules embedded into a transparent medium are studied and related to the experimental observations for pigmented tissues. A strong pulse width dependence of the threshold energy for producing a visible damage to the absorbing granule and the mechanism of the damage is observed. The acoustic impedance mismatch at the interface between the absorbing granule and the surrounding medium is found to define the role of the intragranular fracturing in short pulse laser damage.

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